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13. SUPPLEMENTARY NOTES

14. ABSTRACT

The objective of the present program was to study the structure and response of laminar premixed and nonpremixed flames with emphases on effects of high pressure, flame/flow unsteadiness, and chemistry. Studies on flame dynamics show strong coupling between the intrinsic flamefront hydrodynamic cellular instabilities and the diffusional-thermal cellular or pulsating instabilities, for mixture Lewis numbers that are respectively smaller or larger than unity. Linear and nonlinear stability analyses on diffusion flames show regimes of stability and the influence of heat loss on their boundaries. Studies on combustion chemistry led to the determination of laminar flame speeds of high fidelity at atmospheric and high pressures for CO/H₂ as well as C₂-C₃ mixtures with air, and the counterflow ignition temperatures of dimethyl ether (DME) and 1,3-butadiene, allowing developments of detailed and reduced reaction mechanisms. A mathematical theory and computational algorithm termed directed relation graph was developed and then further improved that allows systematic and rapid determination and thereby elimination of unimportant species and reactions of detailed mechanisms, leading to skeletal mechanisms that are sufficiently small either for computational simulation of complex combustion phenomena. These results are expected to be useful to the general interests of AFOSR in the fundamental and practical issues of flame dynamics and chemical kinetics, turbulent combustion, soot formation, radiative heat transfer, flame extinction, stabilization, flammability, and supersonic combustion.

15. SUBJECT TERMS

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Final Report

PHYSICAL AND CHEMICAL PROCESSES IN FLAMES

(Grant Number: FA9550-04-1-0003)

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SUMMARY/OVERVIEW

The objective of the present program was to study the structure and response of laminar premixed and nonpremixed flames with emphases on effects of high pressure, flame/flow unsteadiness, and chemistry. The investigations were conducted through laser-based experimentation, computational simulation with detailed chemistry and transport descriptions, and advanced mathematical analysis. Phenomena studied include the development and control of intrinsic flamefront instabilities, the acquisition of fundamental flame data of high fidelity, and the development of detailed and simplified chemical kinetic mechanisms.

Studies on flame dynamics show strong coupling between the intrinsic flamefront hydrodynamic cellular instabilities and the diffusional-thermal cellular or pulsating instabilities for mixture Lewis numbers that are, respectively, smaller or larger than unity. Linear and nonlinear stability analyses of diffusion flames show regimes of stability and the influence of heat loss on their boundaries.

Studies of combustion chemistry proceeded in two directions. In the first, laminar flame speeds of high fidelity were determined at atmospheric and high pressures for CO/H₂ as well as C₂-C₃ mixtures with air, allowing scrutiny and improvement of the existing reaction mechanisms. Furthermore, the ignition temperatures of counterflowing dimethyl ether (DME) and 1,3-butadiene against heated air were determined experimentally and used to revise existing detailed mechanisms for their oxidation and the development of the associated reduced mechanisms. In the second direction, a mathematical theory and computational algorithm, termed directed relation graph, was developed and improved further that allows systematic and rapid determination, and thereby elimination, of unimportant species and reactions of detailed mechanisms, leading to skeletal mechanisms that are sufficiently small either for computational simulation of complex combustion phenomena or for further reduction.

These results are expected to be useful to the general interests of AFOSR in the fundamental and practical issues of flame dynamics and chemical kinetics, turbulent combustion, soot formation, radiative heat transfer, flame extinction, stabilization, flammability, and supersonic combustion.

ACCOMPLISHMENT

The research program has two major foci, namely the unsteady dynamics and control of flames, and the chemical kinetics of flames including realistic simulation of their effects. These two foci cover a substantial arena in the current research activities in fundamental combustion and combustion modeling and simulation. Good progress has been made in both endeavors during the program period. Highlights of the accomplishments can be found in the annual Progress Reports submitted to the program director, as well as the journal papers that have appeared in print. Thus only a brief summary of these works are mentioned in the following.

Unsteady Flame Dynamics and Control

Practical combustion situations frequently involve turbulent flames. Under most conditions chemical reactions take place in narrow regions, constituting the so-called laminar flamelets. These laminar flamelets are subjected to the fluctuating shearing action of the turbulent eddies and under severe conditions can be extinguished locally. Furthermore, because of the disparity in the diffusivities of the heat and reactants, the flame front can exhibit intrinsic instability in the forms of cellularity and pulsation of the flame surface. Intrinsic cellular instability also can occur due to the substantial density jump across the flame front through the so-called Landau, or hydrodynamic, instability. The presence of such instabilities can modify the burning rate and possibly even affect the state of extinction. Studies of flame front instability during the program period have assumed two directions, namely high-level computational simulations of premixed flame propagation subjected to the combined effects of hydrodynamic and diffusional-thermal instabilities, and theoretical analyses of intrinsic pulsating instability of diffusion flames, without and with radiative heat loss. The intention is eventually to couple forced and intrinsic instabilities to explore combustion control through resonance. The following section is a synopsis of the results and the understanding gained therein.

Coupled Hydrodynamic and Diffusional-Thermal Instabilities [1, 2]

There are two major modes of intrinsic flamefront instabilities in premixed flame propagation. The first mode is the hydrodynamic instability due to the disparity of the density across the flame surface, and tends to generate cells. The second mode is diffusion-thermal instability due to the disparity between the thermal and mass diffusivities, as characterized by the mixture Lewis number, Le . Specifically, the instability takes the form of cells when $Le < 1$ and pulsations when $Le > 1$. When related to actual fuel-air mixtures, it is well-established that lean hydrogen-air and methane-air are $Le < 1$ mixtures, while their rich counterparts are $Le > 1$ mixtures. Conversely, lean propane-air and mixture of air with the higher hydrocarbons are $Le > 1$ mixtures, while their

rich counterparts are $Le < 1$ mixtures. The richness of the flame response as a mixture changes from being lean to rich or when the fuel changes from methane to the higher hydrocarbons, is quite evident. This complexity of the flamefront instability is enriched further when the two modes of instabilities are coupled. Specifically, for $Le < 1$ flames, the hydrodynamic cells can assume all sizes, while the diffusional-thermal cells are smaller. For $Le > 1$ flames the hydrodynamic cells would be affected by the diffusional-thermal pulsations.

While analytical studies have been performed for the stability boundaries of coupled instabilities, very little has been done on the nonlinear stabilities that describe the evolution of the cells and consequently the flame propagation. The complexity of the phenomena warrants computational simulation with high-order accuracy, which was enabled by using a sixth-order central difference scheme and newly developed non-reflective boundary conditions. The study was further conducted in two components: for $Le < 1$ and > 1 mixtures.

For $Le < 1$ mixtures, results [1] show that the continuous flame evolution can be characterized by several elemental processes, including cell splitting, merging, and lateral movement. All these processes involve coupling between the two modes of instabilities. Since the hydrodynamic effect depends on the scale of the flame interface, the size of domain affects the results. Furthermore, there exists a critical Le , Le_c , such that when $Le < Le_c$, the diffusion-thermal effect aggravates the hydrodynamic instability, cell splitting and merging are accelerated, and the flame cell travels laterally. Cell evolution also induces local extinction which is responsible for leakage of the unburned fuel. If Le is reduced further, for example to $Le = 0.3$, hydrodynamic instability induces a convergent flow and convects the small cell to the trough area. This instability generates small cell shedding, causing the flame to propagate unsteadily with high frequency. On the other hand, hydrodynamic instability is stabilized by the diffusional-thermal effect when $Le > Le_c$, resulting in the steady propagation of a stabilized cellular flame. Hydrodynamic instability can be excited through faster laminar flame speed and larger computational domain, and strong hydrodynamic instability alone can induce cell splitting and merging. No lateral movement is observed if $Le > Le_c$.

For $Le > 1$ mixtures, results [2] in the linear stage of the instability growth show that the growth rate dramatically decreases with increasing Le and that the large activation energy excites the pulsating instability and increases the growth rate of the hydrodynamic instability. In the nonlinear growth stage, there exist regimes of stable cell propagation, periodic pulsating cellular flames, and irregular pulsating cellular flames as the activation energy is increased. Characteristics of these regimes were studied further for the effects of Le on the flame front structure in the regime of stable cell propagation; the effects of flame pulsation on the flow and flame cell structure in the regime of periodic pulsating cellular flame; and the complex pattern formation in the regime of irregular pulsating cellular flame. Unsteady pulsating flames can

propagate faster than the adiabatic flame when the local stretch rate is positive, implying that models based on quasi-steady flame propagation may not predict the behavior of unsteady flames with large Le correctly.

Intrinsic Instabilities and Extinction of Diffusion Flames [3, 4]

While it is generally believed that, unlike premixed flames, diffusion flames are stable in response to perturbations to diffusional-thermal imbalances because the reaction is diffusion controlled, it also is recognized that instabilities could be incited when finite-rate chemistry becomes important near limits of extinction. Indeed, it has been suggested that monitoring the onset of such instabilities could allow the control of flame extinction. We have tackled two problems: a nonlinear analysis of the evolution of pulsating instabilities and a linear analysis of pulsating instabilities in the presence of heat loss. In both analyses we consider the simple geometric configuration of a planar diffusion flame situated in a channel at the interface between a fuel being supplied from one end and oxidant diffusing from a stream at the other end. Lewis numbers are assumed greater than unity in order to focus on pulsating instabilities.

We carried out a bifurcation analysis [3] to derive a nonlinear evolution equation for the amplitude of the perturbation. Our analysis predicts three possible flame responses. The planar flame may be stable, such that perturbations decay to zero. Second, the amplitude of a perturbation eventually can become unbounded in finite time, indicating flame quenching. Finally, our amplitude equation possesses time-periodic (limit cycle) solutions, although we find that this regime cannot be realized for parameter values typical of combustion systems. The various possible burning regimes are mapped in parameter space, and our results are consistent with available experimental and numerical data.

For the second problem [4], a linear stability analysis was conducted to study the onset of near-limit flame oscillation with radiative heat loss using multi-scale activation-energy asymptotics. The oscillatory instability near a *radiation-induced* extinction limit at large Damköhler numbers was identified, in addition to the one near the kinetic limit at small Damköhler numbers. Radiative loss assumed a similar role as varying the thermal diffusivity of the reactants. Thus, flame oscillation near the radiative limit was still thermal-diffusive in nature although it could develop under unity Lewis numbers. The unstable range of Damköhler numbers near the radiative limit showed quite similar parametric dependence on the Lewis numbers of the reactants, Le_F and Le_O , the stoichiometry, ϕ , and the radiative loss as that near the kinetic limit.

Both dependencies increased monotonically with Le_O and ϕ and increased then decreased with Le_F . Increasing radiative loss extended the parameter range under which flame oscillations could develop; however, the oscillations show different dependence on the temperature difference between the supplying reactants. Unless radiative loss approached the maximum value that the system could sustain, flame oscillation near the radiative limit was only possible within a limited range of ΔT , whereas it was promoted monotonically with decreasing ΔT near the kinetic limit. Furthermore, while radiative loss showed small effect on the nondimensional oscillation frequency, the dimensional frequency of flame oscillations near the radiative limit could be substantially smaller than that near the kinetic limit.

Laminar Flame Speeds and Kinetics

Chemical kinetics and transport-supplemented fluid mechanics form the two knowledge bases of combustion. Traditionally, chemical kinetics has been studied in homogeneous systems such as the shock tube and flow reactors. However, since the early 1980s the usefulness of supplementing results from these homogeneous systems with those from diffusion-affected chemical systems has been recognized. Notable global combustion parameters that have assumed essential roles in the development of reaction mechanisms include the laminar burning velocities and the counterflow extinction strain rates for high-temperature kinetics, and the counterflow ignition temperatures for low- to intermediate-temperature kinetics. A major effort of our program is the experimental determination of laminar burning velocities, especially at elevated pressures, and using them to scrutinize and aid in the development of detailed reaction mechanisms.

During the program period we have made useful contributions in this topic along two directions: determination of the laminar flame speeds of a variety of fuels and the development of their reaction mechanisms, and the determination of the counterflow ignition temperatures of a variety of fuels and the development of their reduced reaction mechanisms.

Determination of Laminar Flame Speeds and Development of Detailed Mechanisms [5, 6]

Our first project [5] involved the determination of the laminar flame speeds of CO/H₂/air and CO/H₂/helium mixtures at different equivalence ratios and mixing ratios by the constant pressure spherical flame technique, for pressures up to 40 atmospheres. A kinetic mechanism based on

recently published, evaluated, and calculated reaction rate constants was developed to model these measured laminar flame speeds as well as a wide spectrum of other experimental data. The kinetic model accurately predicted our measured flame speeds and the non-premixed counterflow ignition temperatures determined in our previous study, as well as homogeneous system data from literature such as concentration profiles from flow reactor and ignition delay time from shock tube experiments.

In the second project [6] experimental data were acquired for: (1) the ignition temperatures of nitrogen-diluted ethylene and propylene by counterflowing heated air for various strain rates and system pressures up to 7 atm; (2) the laminar flame speeds of mixtures of air with acetylene, ethylene, ethane, propylene, and propane, deduced from an outwardly propagating spherical flame in our constant-pressure chamber, for extensive ranges of lean-to-rich equivalence ratios and system pressures up to 5 atmospheres. These data subsequently were compared with calculated results using a literature C₁-C₃ mechanism and an ethylene mechanism. Noticeable differences were observed in the comparison for both mechanisms, and sensitivity analyses were conducted to identify the reactions of importance.

Determination of Counterflow Ignition Temperatures and Development of Reduced Mechanisms [7, 8]

We have a separate research program with the Army Research Office to determine the counterflow ignition temperatures of fuels. Through such an activity existing detailed reaction mechanisms can be scrutinized for the low-temperature chemistry, complementing the interest on high-temperature kinetics through flame speed studies in the present program. These detailed mechanisms subsequently also have been reduced using the suite of reduction methodologies that we have developed under the present program. Specifically, the following two projects were conducted.

In the first project [7] the ignition temperature of nitrogen-diluted dimethyl ether (DME) by heated air in counterflow was experimentally determined for DME concentrations from 5.9 to 30%, system pressures from 1.5 to 3.0 atmospheres, and pressure-weighted strain rates from 110 to 170 s⁻¹. These experimental data were compared with two mechanisms that were respectively available in 1998 and 2003, with the latter being a substantially updated version of the former. The comparison showed that while the 1998-mechanism uniformly over-predicted the ignition

temperature, the 2003-mechanism yielded surprisingly good agreement with all experimental data. Sensitivity analysis for the near-ignition state based on both mechanisms identified the deficiencies of the 1998-mechanism, particularly the specifics of the low-temperature cool flame chemistry in effecting ignition at higher temperatures, as the fuel stream was being heated progressively from its cold boundary to the high-temperature ignition region around the hot-stream boundary. The 2003-mechanism, consisting of 79 species and 398 elementary reactions, then was simplified systematically by using the directed relation graph method, to be discussed in the next section, to a skeletal mechanism of 49 species and 251 elementary reactions, which, in turn, was simplified further by using the computational singular perturbation method and the quasi-steady-state species assumption to a reduced mechanism consisting of 33 species and 28 lumped reactions. Both the skeletal and reduced mechanisms mimicked the performance of the detailed mechanism with high accuracy.

In the second project [8] the ignition temperatures of nitrogen-diluted 1,3-butadiene by heated air in counterflow were determined experimentally for pressures up to 5 atmospheres and pressure-weighted strain rates from 100 to 250 s⁻¹. The experimental data were compared with computational results using the mechanism of Laskin *et al.*, showing that, while the overall prediction is approximately within the experimental uncertainty, the mechanism over-predicts ignition temperature by about 25 – 40K, with the differences becoming larger in the high pressure/low temperature region. Sensitivity analyses for the near-ignition states were performed for both reactions and diffusion, which identified the importance of H₂/CO chain reactions, three 1,3-butadiene reaction pathways, and the binary diffusion between 1,3-butadiene and N₂ on ignition. The detailed mechanism, consisting of 94 species and 614 reactions, then was simplified to a skeletal mechanism consisting of 46 species and 297 reactions by using a new reduction algorithm combining directed relation graph and sensitivity analyses. The skeletal mechanism was simplified further to a 30-step reduced mechanism by using computational singular perturbation and quasi-steady-state assumptions. Both the skeletal and reduced mechanisms mimicked the performance of the detailed mechanism with good accuracy in both homogeneous and heterogeneous systems.

Theories and Algorithms for Kinetic Mechanism Reduction [9, 10, 11]

When the present research program was initiated a few years ago, the stated objective was the development of comprehensive detailed mechanisms covering hydrocarbons all the way from methane to the C₇-C₈ range. While this objective is still an important focus, an additional goal has emerged, namely the development of mathematical theories and computational algorithms for the automatic reduction of detailed mechanisms to simpler ones without loss of comprehensiveness. This undertaking was motivated by two considerations. First, detailed mechanisms are simply too large for integration into the computation of combustion flow fields. For example, the class of mechanisms developed by Westbrook and co-workers at the Lawrence Livermore laboratories, consisting of hundreds of species and thousands of reactions, cannot be used even for the calculation of the one-dimensional laminar flame structure and the associated flame speed. Other smaller mechanisms, such as GRI-Mech for methane oxidation, cannot be used for turbulent flame calculations. The second motivation was that the continuing updating of detailed mechanisms as new experimental and *ab initio* computational data becomes available. Obviously it is not reasonable to expect that a manual reduction needs to be performed whenever a new mechanism appears.

Perhaps the most significant contribution that was made in this endeavor during the program period was the formulation of a systematic method, based on graph theory, through which unimportant species and reactions can be eliminated, thereby substantially reducing the size of the mechanism [9]. The approach consists of the generation of skeletal mechanisms from detailed mechanism using directed relation graph (DRG) with specified accuracy requirement, and the subsequent generation of reduced mechanisms from the skeletal mechanisms using computational singular perturbation based on the assumption of quasi-steady-state species. Both stages of generation are guided by the performance of a perfectly stirred reactor (PSR) for high-temperature chemistry and auto-ignition delay for low- to moderately-high-temperature chemistry. The demonstration was performed for a detailed ethylene oxidation mechanism consisting of 70 species and 463 elementary reactions, resulting in a specific skeletal mechanism consisting of 33 species and 205 elementary reactions, and a specific reduced mechanism consisting of 20 species and 16 global reactions. Calculations for laminar flame speeds and nonpremixed counterflow ignition using either the skeletal mechanism or the reduced mechanism show very close agreement with those obtained by using the detailed mechanism over wide parametric ranges of pressures, temperatures, and equivalence ratios.

The algorithm of directed relation graph (DRG) then was extended to overall linear-time operation [10], thereby greatly facilitating the computational effort in mechanism reduction, particularly for those involving large mechanisms. Together with a two-stage reduction strategy

and using the kinetic responses of auto-ignition and PSR with extensive parametric variations as the criteria for eliminating unimportant species, a detailed 561-species n-heptane mechanism and a detailed 857-species iso-octane mechanism were reduced successfully to skeletal mechanisms consisting of 188 and 233 species respectively. These skeletal mechanisms were demonstrated to mimic well the performance of the detailed mechanisms, not only for the auto-ignition and PSR systems based on which the reduced mechanisms were developed, but also for the independent system of a jet-stirred reactor. The accuracy of calculated species concentrations was bounded equivalently by the user-specified error threshold value, and the reduction time for a single reaction state was only about 50 ms for the large iso-octane mechanism.

The conditions for application of the directed relation graph then were analyzed systematically [11]. The existence of quasi steady state species induced no additional restriction to the application of DRG. When there were partial equilibrium reactions, DRG required reactions with fast forward or backward rates to be reversible and the backward rate to be computed through the equilibrium constant. The effect of loss in significant digits in the evaluation of species relations due to substantial cancellation between the forward and backward rates of partial equilibrium reactions was identified, and a criterion for minimum accuracy in sampled reaction states for DRG reduction also was established. The method of DRG then was compared with two methods recently developed for skeletal reduction, one based on computational singular perturbation (CSP) and the other on the directed relation graph with error propagation (DRGEP). Advantages and restrictions of including fast-slow subspace separation in skeletal reduction and the validity of the geometric error propagation model in DRGEP were discussed with examples in the existence of exhausted fast processes.

We also have developed a reduced mechanism for methane oxidation that has been used in the direct numerical simulation of a three-dimensional spatially-developing turbulent slot-burner Bunsen flame [12]. The simulation was performed for three flow through times long enough to achieve statistical stationarity. The turbulence parameters were chosen such that combustion occurred in the thin reaction zones regime of premixed combustion. The data were analyzed to study possible influences of turbulence on the structure of the preheat and reaction zones. The results showed that the mean thickness of the turbulent flame was greater than the corresponding laminar flame. The effects of flow straining and flame front curvature on the mean flame thickness were quantified through conditional means of the thickness and by examining the

balance equation for the evolution of the flame thickness. Finally, a comparison of the conditional mean reaction rate of key species to the laminar reaction rate profiles showed that there was no significant perturbation of the heat release layer.

Miscellaneous Topics of Interest to Aeropropulsion

We have performed two projects that are not part of our proposal but are nevertheless of intrinsic interest to combustion and aeropropulsion. The first [13] was the observation that the cause of the rich-shifting of the adiabatic flame temperature is product dissociation. The influence of this rich shifting permeates combustion phenomena such as the laminar flame speed because of their essential dependence on the adiabatic flame temperature.

The second project was an examination of the concept of flammability limits under the high-pressure environment of internal combustion engines [14] and relating it to limitations on the control of NO_x.

Review Activities [15, 16, 17]

Three review articles were written on some general issues on combustion, with most of the understanding gained through the present program conducted throughout the years. Reference 15 emphasizes the importance of comprehensive description of chemistry in combustion modeling, while Ref. 16 focuses on high-pressure combustion. Reference 17 is the Hottel Lecture delivered at the 31st International Combustion Symposium.

Writing review articles is a major, though essential, undertaking. The P.I. is pleased to have contributed to the literature in this manner.

JOURNAL PUBLICATIONS

Flamefront Instabilities and Control

1. "Coupled hydrodynamic and diffusional-thermal instabilities in flame propagation at sub-unity Lewis numbers," by J. Yuan, Y. Ju and C.K. Law, *Physics of Fluids*, Vol. 17, Art. No. 074106 (2005).
2. "Pulsating and hydrodynamic instabilities at large Lewis numbers," by J. Yuan, Y. Ju and C.K. Law, *Combustion and Flame*, Vol. 144, pp. 386-397 (2005).
3. "Nonlinear oscillations in diffusion flames," by H.Y. Wang, J.K. Bechtold and C.K. Law, *Combustion and Flame*, Vol. 145, pp. 376-389 (2006).
4. "On intrinsic oscillation in radiation-affected diffusion flames," by H.Y. Wang and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 31, pp. 979-987 (2007).

Laminar Flame Speeds and Kinetics

5. "High-pressure laminar flame speeds and kinetic modeling of carbon monoxide/hydrogen combustion," by H.Y. Sun, S.Y. Yang, G. Jomaas, and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 31, pp. 439-446 (2007).
6. "Experimental determination of counterflow ignition temperatures and laminar flame speeds of C₂-C₃ hydrocarbons at atmospheric and elevated pressures," by G. Jomaas, X. L. Zheng, D. L. Zhu, and C. K. Law, *Proceedings of the Combustion Institute*, Vol. 30, pp. 193-200 (2005).
6. "Experimental and computational study of nonpremixed ignition of dimethyl ether in counterflow," by X. L. Zheng, T. F. Lu, C.K. Law, C. K. Westbrook, and H.J. Curran, *Proceedings of the Combustion Institute*, Vol. 30, pp. 1101-1109 (2005).
8. "Experimental counterflow ignition temperatures and reaction mechanisms of 1,3-butadiene," by X.L. Zheng, T.F. Lu and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 31, pp. 367-375 (2007).

Theories and Algorithms for Kinetic Mechanism Reduction

9. "A directed relation graph method for mechanism reduction," by T. F. Lu and C. K. Law, *Proceedings of the Combustion Institute*, Vol. 30, pp. 1333-1341 (2005).
10. "Linear-time reduction of large kinetic mechanisms with directed relation graph: n-heptane and iso-octane," by T. F. Lu and C. K. Law, *Combustion and Flame*, Vol. 144, pp. 24-36, (2005).

11. "On the applicability of directed relation graph to the reduction of reaction mechanisms," by T. F. Lu and C. K. Law, *Combustion and Flame*, Vol. 146, pp. 472-483 (2006).
12. "Structure of a spatially-developing turbulent lean methane-air Bunsen flame," by R. Sankaran, E.R. Hawkes, J.H. Chen, T.F. Lu and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 31, pp. 1291-1298 (2007).

Miscellaneous Topics of Interest to Aeropropulsion

13. "On the off-stoichiometric peaking of adiabatic flame temperature with equivalence ratio", by C.K. Law, A. Makino and T.F. Lu, *Combustion and Flame*, Vol. 145, pp. 808-819 (2006).
14. "An assessment of the lean flammability limits of CH₄/air and C₃H₈/air mixtures at engine-like conditions," by F.N. Egolfopoulos, A.T. Holley and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 31, pp. 3015-3022 (2007).

Review Articles

15. "Comprehensive description of chemistry in combustion modeling," by C. K. Law, *Combustion Science and Technology*, Vol. 177, pp. 1-26 (2005).
16. "Propagation, structure, and limit phenomena of laminar flames at elevated pressures," by C.K. Law, *Combustion Science and Technology*, Vol. 178, pp. 335-360 (2006).
17. "Combustion at a crossroads: status and prospects," by C.K. Law, *Proceeding of the Combustion Institute*, Vol. 31, pp. 1-29 (2007).

PREPRINTS AND REPORTS

1. "Approaches to mechanism reduction for hydrocarbon oxidation: ethylene," by T. F. Lu and C. K. Law, Paper No. AIAA 2004-1326, 42nd Aerospace Sciences Meeting, Reno, NV, Jan. 5-8, 2004.
2. "Nonlinear analysis of pulsating instabilities in diffusion flame," by H.Y.Wang, J.K. Bechtold, and C.K. Law, Paper No. AIAA 2005-0544, 43rd Aerospace Sciences Meeting, Reno, NV, Jan. 10-13, 2005.

3. "Linear time reduction of large kinetic mechanisms with directed relation graph:n-heptane and iso-octane," T.F. Lu and C.K. Law, Paper No. C13, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
4. "Thermochemical and kinetic analyses on oxidation of isobutenyl radical and 2-hydroperoxymethyl-2-propenyl radical," X.L. Zheng, H.Y. Sun, and C.K. Law Paper No. C20, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
5. "Experimental determination of laminar flame speeds and kinetic modeling of hydrogen/chlorine combustion," J. C. Leylegian, H.Y. Sun, and C.K. Law, Paper No. C40, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
6. "Pulsating and hydrodynamic instabilities for large Lewis number flames," J. Yuan, Y. Ju, and C.K. Law, Paper No. F10, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
7. "On the off-stoichiometric peaking of adiabatic flame temperatures," C.K. Law, A. Makino, and T.F. Lu, Paper No. F13, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
8. "Forced oscillation in diffusion flames near resonance," H.Y. Wang, J.K. Bechtold, and C.K. Law, Paper No. F26, 4th Joint Meeting of the US Sections of the Combustion Institute, Philadelphia, Pa, March 20-23, 2005.
9. "Flame propagation with hydrodynamic and body-force instabilities in vortical flows," by K.L. Pan, C.K. Law, and C.H. Wang, the Sixth Asian Computational Fluid Dynamics Conference, Taiwan, Oct. 24-27, 2005.
10. "Ignition of the butene isomers: an experimental and kinetics study," by X.L. Zheng, H.Y. Sun, and C.K. Law, Paper No. 05F-9, Fall Technical Meeting of the Western States Section of the Combustion Institute, Stanford, CA, Oct. 17-18, 2005.
11. "Large eddy simulation of soot formation in turbulent premixed flames," H. El-Asrag, S. Menon, T.F. Lu, and C.K. Law, AIAA Paper 2006-0153, 44th Aerospace Sciences Meeting, Reno, NV, Jan. 9-12, 2006.
12. "Study of turbulent premixed flame thickness using direct numerical simulation," R. Sankaran, E. Hawkes, J.H. Chen, T.F. Lu, and C.K. Law, AIAA Paper 2006-0165, 44th Aerospace Sciences Meeting, Reno, NV, Jan. 9-12, 2006.
13. "Simulations of cavity-stabilized flames in supersonic flows using reduced chemical kinetic mechanisms," by J.W. Liu, C.J. Tam, T.F. Lu, and C.K. Law, AIAA paper 2006-4862, 42nd Joint Propulsion Conference, Sacramento, CA, July 9-12, 2006.

PRESENTATIONS

Keynote and Named Lectures

- 1 "Combustion characteristics of energetic liquid propellants," National Aerospace Conference, National Cheng Kung University, Tainan, Taiwan, Dec. 19, 2003. * Keynote Lecture*
- 2 "From atomic to cosmic: A panoramic view of combustion," Eighth Aisinjiro-Soo Lecture, University of Illinois, Urban-Champaign, Oct. 12, 2004.
- 3 "The role of combustion in hydrogen economy," 7th Asian-Pacific Symposium on Combustion and Energy Utilization, Hong Kong, Dec. 15-17, 2004. * Keynote Lecture*
- 4 "The role of combustion in hydrogen economy," International Green Energy Conference, University of Waterloo, Waterloo, Canada, June 13-15, 2005. * Keynote Lecture*
- 5 "Fifty years of magnificent combustion research in Japan," 43rd Symposium (Japanese) on Combustion, Tokyo, Japan, Dec. 5-7, 2005. * Plenary Lecture*
- 6 "Combustion at a crossroads: status and prospects," Hottel Lecture, 31st International Symposium on Combustion, Heidelberg, Germany, August 7-11, 2006. * Plenary Lecture*
- 7 "Dynamics of droplet collision," Technical Meeting of the Institute for Liquid Atomization and Spray Systems (ILASS), Chicago, IL, May 15-17, 2007. * Keynote Lecture*
- 8 "The role of combustion in climate change and energy sustainability," Sixth Asian-Pacific Conference on Combustion (ASPACC 07), Nagoya, Japan, May 21-23, 2007. **Conference Opening Lecture**
- 9 "The role of combustion in aerospace and space studies," I.I. Glass Memorial Lecture, University of Toronto Institute for Aerospace Studies, Toronto, Canada, June 7, 2007.

Invited Departmental Seminars and Conference Session Talks

1. "Some thoughts and action items in mechanism development for combustion applications," Workshop on the Simulation of the Combustion of Real Fuels, NIST, Gaithersburg, MD, Sept. 4-5, 2003.
2. "Properties of propane combustion," Strategic Planning Meeting, British Petroleum Corp., Chicago, IL, Nov. 20, 2003.
3. "Comprehensive description of chemistry in combustion modeling," Symposium on the Advancements in Combustion Theory, University of California at San Diego, La Jolla, CA, Jan. 10, 2004.
4. "Some recent contributions to combustion chemistry, flame theory, and droplet dynamics," NIST, Gaithersburg, MD, May 5, 2004.

5. "Role of laminar flamelets and reduced chemistry in turbulent flame modeling and simulation," Symposium of Advanced Combustion Modeling, Cranfield University, England, Sept. 21, 2004.
6. "Ignition kinetics and flame dynamics in hydrogen combustion," Department of Mechanical Engineering, Pennsylvania State University, September 30, 2004.
7. "From atomic to cosmic: A panoramic view of combustion," College of Engineering, National Central University, Jhongli, Taiwan, October 27, 2004.
8. "Frontiers of combustion: from microgravity to microengines," Department of Aerospace Engineering, Iowa State University, Ames, Iowa, November 4, 2004.
9. "From atoms to the cosmos: a panoramic view of combustion," Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, March 25, 2005.
10. "Basic needs in scramjet lean blowout," Workshop on Scramjet Lean Blowout, JANNAF Conference, Charleston, S.C., June 16, 2005.
11. "Some issues on combustion and chemistry in high-energy-density fuels," DARPA Workshop on Future of Military Logistic Fuels, Rice University, Houston, TX, August 30, 2005.
12. "The role of combustion in hydrogen economy," Department of Mechanical Engineering, University of Connecticut, Storrs, Ct., September 30, 2005.
13. "Ignition kinetics and flame dynamics in hydrogen combustion," Workshop on Research Frontiers for Combustion in Hydrogen Economy, National Science Foundation, March 9-10, 2006.
14. "Physical and experimental perspectives in flamefront instability," Third Conference in Frontiers in Applied and Computational Mathematics, New Jersey Institute of Technology, Newark, NJ, May 15-16, 2006.
15. "The role of combustion in global warming," Department of Mechanical Engineering, University of Hawaii, Manoa, HI, September 7, 2006.
16. "Development of computationally accessible reaction mechanisms in chemical propulsion," JANNAF Propulsion Conference, San Diego, CA, Dec. 4-8, 2006.
17. "Some aspects of combustion at elevated pressures," JANNAF Propulsion Conference, San Diego, CA, Dec. 4-8, 2006.
18. "Ignition kinetics and flame dynamics in hydrogen combustion," School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA, December 19, 2006.
19. "From Atomic to Cosmic: A panoramic view of combustion," School of Engineering Open Lecture, Hong Kong Polytechnic University, Hong Kong, April 13, 2007.

PERSONNEL

Principal Investigator

C.K. Law

Senior Collaborators

J.K. Bechtold (New Jersey Institute of Technology)
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A. Makino (Shizuoka University, Japan)
Y. Ju (Princeton)

Post-Doctoral Fellows and Research Staff

T.F. Lu
H.Y. Sun
S.Y. Yang
D.L. Zhu

Graduate Students

G. Jomaas (Ph.D. student)
H.Y. Wang (Ph.D. student)
J. Yuan (Ph.D. 2006)
X.L. Zheng (Ph.D. 2006)

SIGNIFICANT INTERACTIONS

1. **Contact:** The Dow chemical Company; Albert Harvey; (225) 353-4035

Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation chemistry

Applications: In-house code development and use.
2. **Contact:** United Technology Research Corp.; M.D. Colket; (860) 610-7481

Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation chemistry

Applications: In-house code development and use
3. **Contact:** Fluent, Inc.; Graham Goldin; (800) 445-4454

Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation with NO_x formation

Applications: Commercially available code for engine and burner simulation
4. **Contact:** Rolls Royce; M. S. Anand, 317- 230-2828

Results: Use of comprehensively validated reduced chemical kinetic mechanism allows improved description of complex species and velocity fields

Applications: Realistic simulation of combustors, especially predictions of pollutant Formation
5. **Contact:** Combustion Research and Flow Technologies; S. Arunajatesan, 215-766-1520

Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation chemistry with NO_x formation.

Applications: Realistic simulation of combustors, especially predictions of pollutant formation